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Hydrogenic impurity, external electric and magnetic fields effects on the nonlinear optical properties of a multi-layer spherical quantum dot

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ABSTRACT

In this work, effects of an on-center hydrogenic impurity, external electric and magnetic fields on the optical rectification coefficient (ORC), second and third harmonic generations (SHG and THG) of a multi-layer spherical quantum dot (MLSQD) are studied. Energy eigenvalues and eigenvectors are calculated using the direct matrix diagonalization method and optical properties are obtained using the compact density matrix approach. Our results reveal that the hydrogenic impurity and external fields have a great influence on these optical quantities. Hydrogenic impurity reduces the magnitude of the resonant peaks and shifts them to the higher energies. An increase in the magnetic (electric) field, leads to increase (decrease) the interval energies and the dipole moment matrix elements. Therefore, resonant peaks of these optical quantities find an obvious blue (red) shift and their magnitudes enhance (diminish) with increasing the external magnetic (electric) field. © 2016 Elsevier Ltd. All rights reserved.

1. Introduction

Recent studies show that the decrease in dimensionality of semiconductors can increase, in certain conditions, their nonlinearities [1]. So there are many investigations focused on the nonlinear optical properties in nano-structures such as quantum wells, wires and dots. Among these structures, nonlinear optical properties of zero-dimensional nano-structures (in which, charge carriers motion has been limited at all sides of spatial), known as quantum dots (QDs), have attracted a great deal of attention due to particular applications and usage as a probe for the electronic structure of mesoscopic media.

Three dimensional nano-scale confinement of electrons in semiconductor QDs leads to the formation of atomic-like discrete energy levels and makes novel physical properties. Thus this type of nano-structures are interesting candidates for high-performance optoelectronic devices [2–6]. Furthermore, because of sensitivity on external fields and other agents, semiconductors QDs have attracted much attention to study their optical properties and electronic structures. There are a lot of studies about the effects of donor impurities, hydrostatic pressure, temperature and external fields on the optical properties of semiconductor QDs [7–21].

Furthermore, coreshell or multilayered spherical quantum dots (MLSQDs) motivated the attention of many researchers, in recent years [22–34]. With the use of effective mass approximation and a self-consistent approach, Salini and co-workers [30] calculated the electronic and optical properties of an exciton in a MLSQD. Aktürk et al. [31], have studied the electronic and

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optical properties of the exciton, the biexciton and charged excitons in a multi-shell quantum dot, by solving the Poisson-Schrödinger equations self-consistently in the Hartree approximation. Effects of the shell thickness, impurity, and dielectric environment on the linear and nonlinear optical absorption coefficients and refractive index changes in ZnO/ZnS core shell quantum dot and ZnS/ZnO inverted core shell quantum dot, have been investigated by zeng et al. [32]. Based on the fourth-order Runge-Kutta method, Karimi et al. [33] calculated the energy eigenvalues and studied the simultaneous effects of the geometrical size, hydrogenic impurity, hydrostatic pressure, and temperature on the intersubband optical absorption coefficients and refractive index changes of a MLSQD. Using the effective mass approximation and the shooting method, Taş and Şahin [34] investigated the inter-sublevel optical properties of a core/shell/well/shell spherical QD with and without considering the impurity effects.

In our recent paper we investigated the effect of hydrogenic impurity and external fields on the electronic structure, optical absorption coefficients and refractive index changes of a MLSQD [35]. Therefore, in the present work, we have studied the effects of external electric and magnetic fields on the second and the third order nonlinear optical properties of an electron bound to an impurity confined in a MLSQD.

The outline of the paper is as follows: In Section 2, we review and summarize the formalism of the electronic structure and optical properties of the system. Section 3 is allocated to the numerical calculation for the optical nonlinearities such as ORC, SHG and THG. Section 4 illustrates the conclusions of the article.

2. Theory

Based on the effective Rydberg units, Hamiltonian of a system consisting of an on-center hydrogenic impurity inside a MLSQD (Fig. 1) in the presence of external electric and magnetic fields, which directed along the *z* direction, can be written as

$$H = -\nabla^2 + V(r) - \frac{2}{r} + \gamma L_z + \frac{1}{4}\gamma^2 r^2 \sin^2 \theta - \eta r \cos \theta$$
⁽¹⁾

where, $\gamma = eB\hbar/2m^*cR_y^*$ is the dimensionless measure of the magnetic field. L_z is the *z*-component of the angular momentum operator. *e*, m^* and *c* are the elementary charge, the effective mass of electron and the speed of light, respectively. $\eta = ea_B^*F/R_y^*$ is the dimensionless measure of the electric field (*F* is the strength of electric field). $a_B^* = e\hbar^2/(m^*e^2)$ and $R_y^* = e^2/2ea_B^*$ are respectively, the effective Bohr radius and Rydberg energy that used as the length and energy units. Here ε is the dielectric constant and the confinement potential of the MLSQD, *V*(*r*), is given by



Fig. 1. Schematic representation of a multilayered spherical quantum dot and its radial potential profile.

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